

Quantum and thermal fluctuations in the SU(N) Heisenberg spin-glass model near the quantum critical point

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We solve for the SU(N) Heisenberg spin-glass in the limit of large N focusing on small S and T . We study the effect of quantum and thermal fluctuations in the frequency dependent response function and observed interesting transfers of spectral weight. We compute the T -dependence of the order parameter and the specific heat and find an unusual T^2 behavior for the latter at low temperatures in the spin-glass phase. We find a remarkable qualitative agreement with various experiments on the quantum frustrated magnet $\text{SrCr}_9\text{Ga}_{12-9p}\text{O}_{19}$.

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Disordered quantum magnets are fascinating systems. The understanding of the interplay between disorder, quantum and thermal fluctuations remains among the most challenging problems of condensed matter physics [1–4]. These three aspects are always present to some extent in experiments on real systems, therefore a clear understanding of their interplay is very desirable. In systems where disorder is relevant we usually encounter the phenomenology of slow dynamics that is associated with glassy states. When quantum fluctuations become important the phases with glassy orders can be driven to more conventional phases through interesting quantum phase transitions [5]. One example that is capturing the interest of experimentalist and theorist alike is $\text{LiHo}_x\text{Y}_{1-x}\text{F}_4$ which is a dipolar coupled random magnet [6] and has been recently the focus of beautiful experiments [7] where quantum fluctuations are introduced and controlled by means of a transverse magnetic field. An other example, and perhaps the archetype of frustrated quantum magnets, is the bi-layer Kagomé lattice $\text{SrCr}_9\text{Ga}_{12-9p}\text{O}_{19}$ (SCGO) that only becomes a spin-glass at the low temperature of about 5K. This compound has been thoroughly investigated over the years [8–12] and, in sharp contrast to ordinary classical spin-glass system, exhibits some unusual remarkable features that are associated with strong quantum fluctuations: The magnetic fluctuation spectrum, $\chi''(\omega)$, is found to vanish linearly in ω at low frequencies [10] and the specific heat is proportional to T^2 [9]. On the theoretical side, these observations have remained largely unaccounted for.

The progress in the understanding models of disordered quantum magnets in finite dimensions is rather slow. In fact, a great deal of our knowledge still relies on solutions of systems with long-ranged interactions. These mean-field models are appealing because they are mathematically more tractable while retaining much of the physics associated with slow dynamics. It is worth pointing out that in many actual systems, such as $\text{LiHo}_x\text{Y}_{1-x}\text{F}_4$ that is an insulator, the magnetic interactions do have power-law decay, thus each individ-

ual spin interacts with others well beyond their nearest neighbours [6].

Among the simplest mean field models for quantum spin-glasses, the quantum version of the Sherrington-Kirkpatrick (SK) model received a great deal of attention. It is a Heisenberg model with gaussianly distributed random interactions between all pair of spins in the lattice. The model was first considered by Bray and Moore [13] and they predicted a spin-glass phase at low temperature, substantially reduced from the usual (Ising) version of the SK model. Further progress was prevented because replica symmetry broken solutions were expected at low T . Later, Sachdev and Ye introduced a generalization of the model to SU(N) spins which could be studied in the large N limit [14]. They found a very interesting spin liquid phase down to $T = 0$. In more recent work on this model, a generalized phase diagram as a function of T and S was obtained using a bosonic representation [15–17]. The spin quantum number S can be thought of a parameter that controls the strength of the quantum fluctuations. For $S \rightarrow \infty$ one goes to the “classical” limit while for small S the quantum fluctuations are strongest. A low temperature spin-glass phase was found for all non zero S and $T_g \sim S^2$ at large S [15–17]. Remarkably, the spin-liquid phase was also found at very low spin S [14–16]. Therefore, quantum fluctuations can drive the model through an interesting quantum critical point between a spin-liquid state at $S \rightarrow 0$ and a quantum spin-glass for finite S .

Recent numerical studies based on quantum Monte Carlo [18] and exact diagonalization [19,20] techniques for the SU(2) model have validated some aspects of previous investigations.

The goal of the present work is to focus on the different roles played by quantum and thermal fluctuations in the SU(N) SK model within the quantum critical regime. We obtain the detailed behavior of the dynamical spin susceptibility for small S and T , both in the paramagnetic (PM) and spin-glass (SG) phases. We find interesting transfers of spectral weights in the magnetic response.

We also find that the spin-glass order parameter has a simple temperature behavior at small S and obtain the correct specific heat at low temperatures. In addition, we discuss the remarkable qualitative agreement that we find between our model solutions and the experimental results in the SCGO compound found that we mentioned above.

The model Hamiltonian is

$$H = \frac{1}{\sqrt{NN}} \sum_{i < j} J_{ij} \vec{S}_i \cdot \vec{S}_j, \quad (1)$$

where the magnetic exchange couplings J_{ij} are independent, quenched random variables distributed according to a Gaussian distribution where J is the variance and the unit of energy. As already pointed out by Bray and Moore [13], one uses the replica trick to average over the disorder [2] and the lattice infinite-range model maps exactly onto a *self-consistent single site model* with the action (in imaginary time τ , with β the inverse temperature) :

$$S_{eff} = S_B - \frac{J^2}{2N} \int_0^\beta d\tau d\tau' Q^{ab}(\tau - \tau') \vec{S}^a(\tau) \cdot \vec{S}^b(\tau') \quad (2)$$

and the self-consistency condition

$$Q^{ab}(\tau - \tau') = \frac{1}{N^2} \langle \vec{S}^a(\tau) \cdot \vec{S}^b(\tau') \rangle_{S_{eff}} \quad (3)$$

where $a, b = 1, \dots, n$ denote the replica indices (the limit $n \rightarrow 0$ has to be taken later) and S_B is the Berry phase of the spin [14]. Due to the time-dependence, the solution of these mean-field equations remains a very difficult problem for $N = 2$, even in the paramagnetic phase [18].

We shall use the bosonic representation [14–17] for the spin operators where S is represented with Schwinger bosons b by $S_{\alpha\beta} = b_\alpha^\dagger b_\beta - S\delta_{\alpha\beta}$, with the constraint $\sum_\alpha b_\alpha^\dagger b_\alpha = SN$ ($0 \leq S$). In the language of Young tableaux, these representations are described by one line of length SN . They are a natural generalization of an $SU(2)$ spin of size S .

In the $N \rightarrow \infty$ limit, the mean field self-consistent model (2-3) reduces to an integral equation for the Green's function of the boson $G_b^{ab}(\tau) \equiv -\langle T b^a(\tau) b^{\dagger b}(0) \rangle$ where the bar denotes the average over disorder and the brackets the thermal average [14] :

$$(G_b^{-1})^{ab}(i\nu_n) = i\nu_n \delta_{ab} + \lambda^a \delta_{ab} - \Sigma_b^{ab}(i\nu_n) \quad (4)$$

$$\Sigma_b^{ab}(\tau) = J^2 (G_b^{ab}(\tau))^2 G_b^{ab}(-\tau) \quad (5)$$

$$G_b^{aa}(\tau = 0^-) = -S \quad (6)$$

The *local* spin susceptibility $\chi_{loc}(\tau) = \langle S(\tau)S(0) \rangle$ is given in the large N limit by $\chi_{loc}(\tau) = G_b^{aa}(\tau)G_b^{aa}(-\tau)$

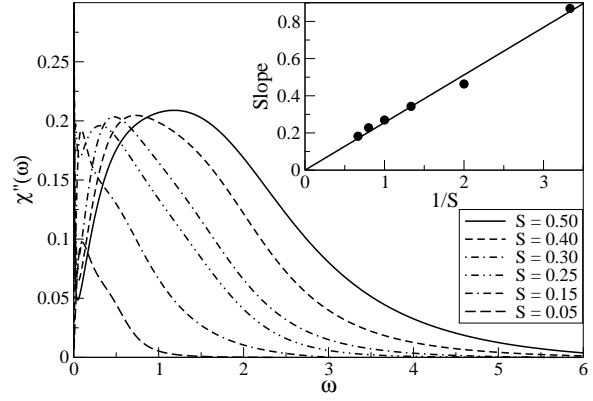


FIG. 1. The imaginary part of the dynamical spin susceptibility $\chi''(\omega)$ as a function of ω for various values of S at $T = 0.04$.

In the spin glass phase it is enough to perform a one step symmetry broken solution [15–17]. Equations (4-6) were solved self-consistently on the Matsubara axis. To obtain the imaginary part of the ω -dependent dynamical response $\chi''_{loc}(\omega)$, the solutions were analytically continued to the real axis using a method based on Padé approximants [21]. The general form of the spin susceptibility can be written as $\chi''_{loc}(\omega) = q_{EA}\delta(\omega) + \chi''_{reg}(\omega)$ where q_{EA} is the spin glass order parameter.

In Fig. 1 we show results for $\chi''_{reg}(\omega)$ at low $T=0.04$ and several values of S across the PM-SG boundary. At this T , the critical S is found at $S \approx 0.28$. We observe a qualitative change in the regular part of the response as S is increased. At low S , in the PM phase, the susceptibility shows the finite temperature spin liquid behavior, obeying $\chi''(\omega) \sim \tanh(\omega/2T)$ for ω small. On the other hand, as S increases and the system goes into the SG phase and $\chi''_{reg}(\omega)$ opens a pseudogap. The thermal excitations become gradually less important and a linear in ω behavior shows up clearly. In fact, we find that the low frequency behavior is proportional to ω/S (inset). This is consistent with the large S solution obtained in [15].

We now turn to the role of thermal fluctuations for fixed $S = 1/2$ that enables comparisons to numerical results obtained in the $SU(2)$ model [18–20]. The freezing temperature is found at $T_g \approx 0.133$ in good agreement with all previous estimates [13,18–20]. We start at low $T = 0.05$ well in the spin-glass phase. In Fig. 2 we show the susceptibility with clean pseudogap $\sim \omega$ behavior at low ω (the $\delta(\omega)$ is not shown for clarity). As T is increased, one observes that excitations gradually fill the pseudogap with a narrow low frequency feature that peaks at $\omega \sim \mathcal{O}(T)$. These excitations come from the gradual melting of the frozen spins, i.e., from the δ -function part. Another interesting effect that one observes is that spectral weight from *high* frequencies of order J is transferred down to the pseudogap. The interpretation of this is that when spins are frozen in the

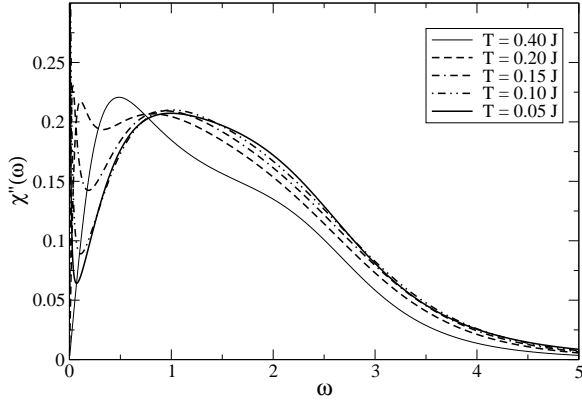


FIG. 2. The imaginary part of the dynamical spin susceptibility $\chi''(\omega)$ as a function of ω for various values of T at $S = 0.5$. Below $T_g \approx 0.133$ the system is in the SG phase and $\chi''(\omega)$ develops a delta function part at $\omega = 0$ that is not shown for clarity.

spin glass state, they still have a fast motion of precession around the axis of their local frozen field. That motion originates a contribution to the susceptibility at $\omega \sim \mathcal{O}(J)$ with a strength proportional to the frozen fraction, i.e., to the order parameter q_{EA} . As T increases, the spins (and thus their local field) melt, so the contribution from the motion of precession gradually decreases and merges with the excitations of order T that now fill the pseudogap. We may point out that this behavior is qualitatively similar to the results obtained from exact diagonalization of small $SU(2)$ clusters [20].

As T is further increased one enters the PM phase and the melted peak fully merges with the higher frequency part of $\chi''(\omega)$ and there is no more a clear separation of energy scales. In this quantum disordered regime the low frequency behaviour of $\chi''(\omega)$ is $\propto \tanh(\omega/2T)$ as in the spin-liquid state [14].

Thus we have seen that the regular part of the response begins at low T in the SG phase with a clean and linear in ω pseudo-gap, then above T_g the gap becomes thermally filled down to very low frequencies, and finally when T is well above T_g the pseudo-gap clears up again displaying once more a linear in ω behavior. We find remarkable that this unusual evolution is qualitatively identical to that reported from neutron experiments in SCSG (cf. Fig.3 of Ref. [10]). Moreover, the neutrons have also revealed that the spatial correlations are extremely short ($\sim 2.5\text{\AA}$) which may render additional justification to the relevance of the present mean-field theory results.

In order to better appreciate the evolution of the transfers of spectral weight at low frequencies and for small T , it is useful to consider the spectral density, defined by $\rho(\omega) = \chi''_{loc}(\omega)/(e^{-\beta\omega} - 1)$ that obeys the sum-rule $\int \rho_{reg}(\omega)d\omega + q_{EA} = S(S+1)$. The spectral density at different temperatures is shown in Fig. 3 where the intensity of the delta function part is denoted by the height of

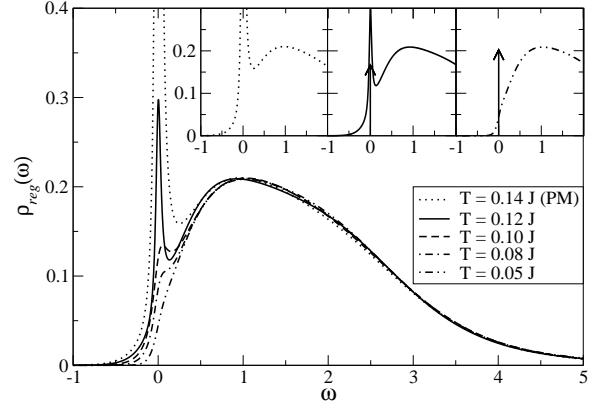


FIG. 3. The regular part of spectral density function $\rho(\omega)$ as a function of ω for various values of T at $S = 1/2$. Below $T_g \approx 0.133$ the system is in the SG phase. The inset shows $\rho(\omega)$ in the PM phase (left), entering the SG phase (center) and at low T within the SG (right). The height of the arrow indicates the spectral intensity of the delta part at the origin.

the arrow (see inset) and can be thought as the fraction of frozen spins. In the main panel we show the regular part of the spectral density that has a broad background contribution that remains almost temperature independent. Most of the T -dependence occurs at the low frequencies where a rather narrow peak is present. At the higher temperature, in the PM phase there is no delta function contribution, however the large peak at small ω indicates that a portion of the degrees of freedom actually got slowed down (left panel of inset). As T is lowered, the system enters the SG phase and the peak becomes narrower and loses weight. A δ -function contribution thus emerges as some of the slow spins become frozen (central panel of inset). When T is further lowered towards $T = 0$ we observe how the resonance loses all its weight that gets transferred to the δ part (right panel of inset). The strong quantum fluctuations are responsible for the large remanent background spectral density that corresponds to a large fraction of spins remaining disordered.

The results for the spin-glass order parameter $q_{EA}(T)$ are shown in the inset of Fig. 4. The behavior at moderate and large values of S was previously investigated in Ref. [16]. We focus here in the small S and T regime and find that the order parameter obeys the simple form

$$q_{EA}(T) = q_{EA}(T = 0) - \alpha T^2 \quad (7)$$

with α a constant, which is similar to the solution of the SK model [1,22]. We also find that the value of q_{EA} at $T = 0$ and its jump at $T_g(S)$ are strongly reduced by quantum fluctuations when $S \rightarrow 0$. In fact, the latter vanishes faster than S^3 in contrast to the quadratic dependence at large S [16]. It is interesting to note the good agreement between $q_{EA}(T = 0) \approx 0.20$ for $S = 1/2$ with the corresponding estimate $q_{EA}(T = 0) \approx 0.18$ obtained in an exact diagonalization study of the $SU(2)$ model [20].

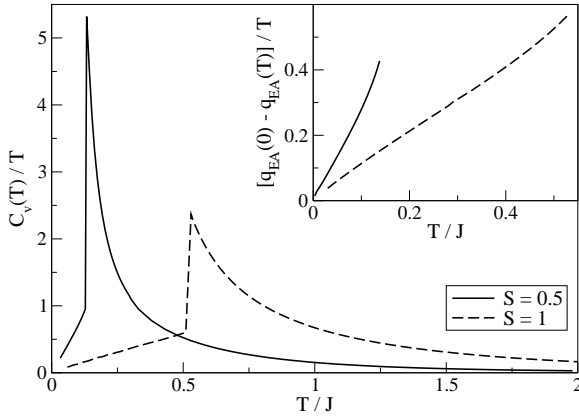


FIG. 4. The specific heat $C_v(T)/T$ for $S = 1/2$ and 1. Inset: The SG order parameter $[q_{EA}(T=0) - q_{EA}(T)]/T$ as a function of T for the same values of S .

Possibly more significant is to mention that a frozen moment of only 20% of the total possible elastic value was observed in neutron scattering on SCGO [10,11].

Finally we turn to the specific heat C_v . In earlier work [15], it was argued that the specific heat is linear in T at low temperatures within the SG phase. We calculated the specific heat in the whole range of S values, with particular care in the small S regime. In contrast to previous results [23], we find that the behavior within the SG phase at low T has the form $C_v(T) \propto T^2$ as is shown in Fig. 4. This result can be justified by the following argument: The energy of the system is given by,

$$E(T) = -\frac{J^2}{2} \int_0^\beta d\tau Q^{ab}(\tau) Q^{ab}(-\tau). \quad (8)$$

Writing this expression in the SG phase in terms of the one-step replica symmetry broken solution [15] and inserting the functional form of the order parameter (7), one finds that the lowest order terms in the T -expansion of $E(T)$ are proportional to T^{-1} , T^1 and T^3 . It is not hard to check that the coefficient of the divergent T^{-1} term exactly cancels. On the other hand, the linear term should also vanish as otherwise the groundstate would have extensive remanent entropy. Therefore, one may expect that the first non vanishing contribution to the energy at low T is proportional to T^3 , which implies a quadratic behavior for $C_v(T)$ as is in fact borne out of our calculations. While ordinary spin-glasses usually show a linear in T specific heat, we find remarkable that the unusual T^2 behavior that we obtain was indeed observed among the early investigations of the spin-glass state of the SCGO compound [9] that pointed to the important role that quantum fluctuations might play in that compound.

To conclude, we have solved for the behavior of the Heisenberg $SU(N)$ spin-glass in the limit of large N and

investigated in detail the parameter region of small S and T close to the quantum critical point of the model. We observed the qualitatively different role played by quantum and thermal fluctuations through their effect on the transfers of spectral weight in the dynamical response functions. We obtained the functional form of the order parameter and present an argument to support the finding of an unusual quadratic behavior of the specific heat at low temperature within the spin glass phase. We find a very interesting qualitative agreement with various experimental findings in the SCGO compound one of the most thoroughly investigated quantum spin-glass system. Extensions of our work to incorporate a more realistic geometric structure might be interesting routes for future research.

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